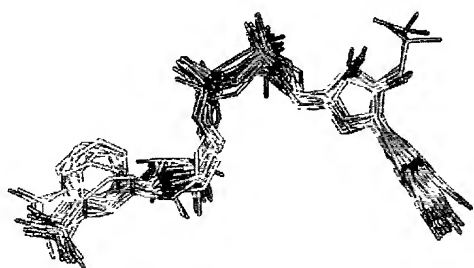
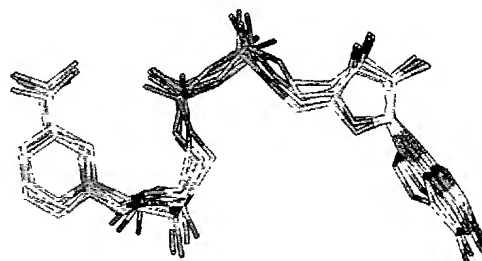


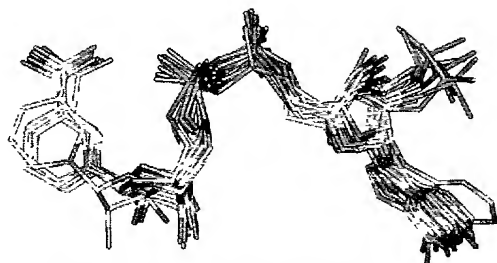
Dehydrogenase Pharmacoclusters



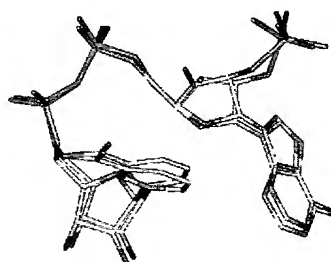
Pharmacocluster 1



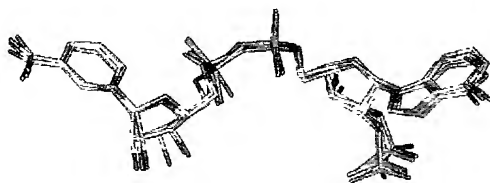
Pharmacocluster 2



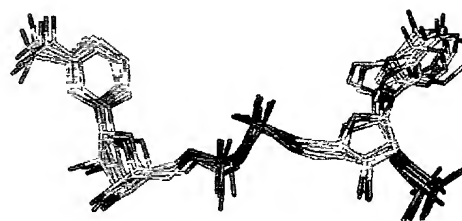
Pharmacocluster 3



Pharmacocluster 4



Pharmacocluster 5



Pharmacocluster 6

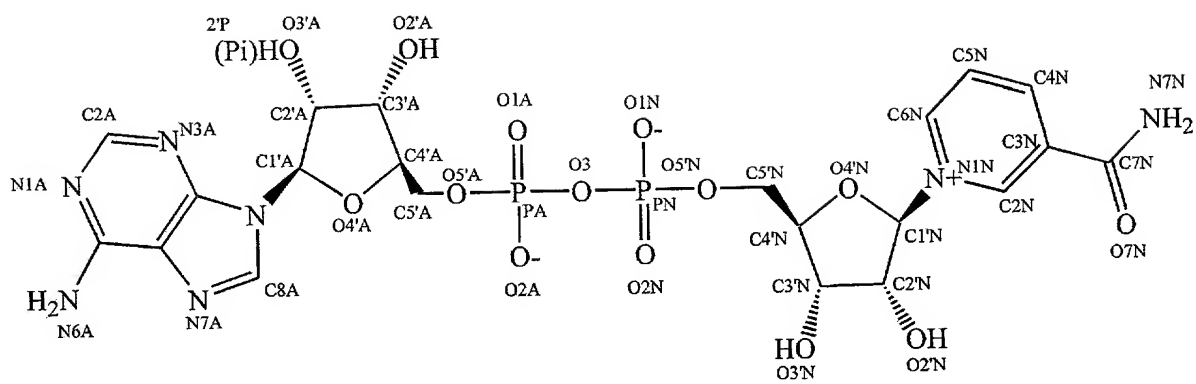


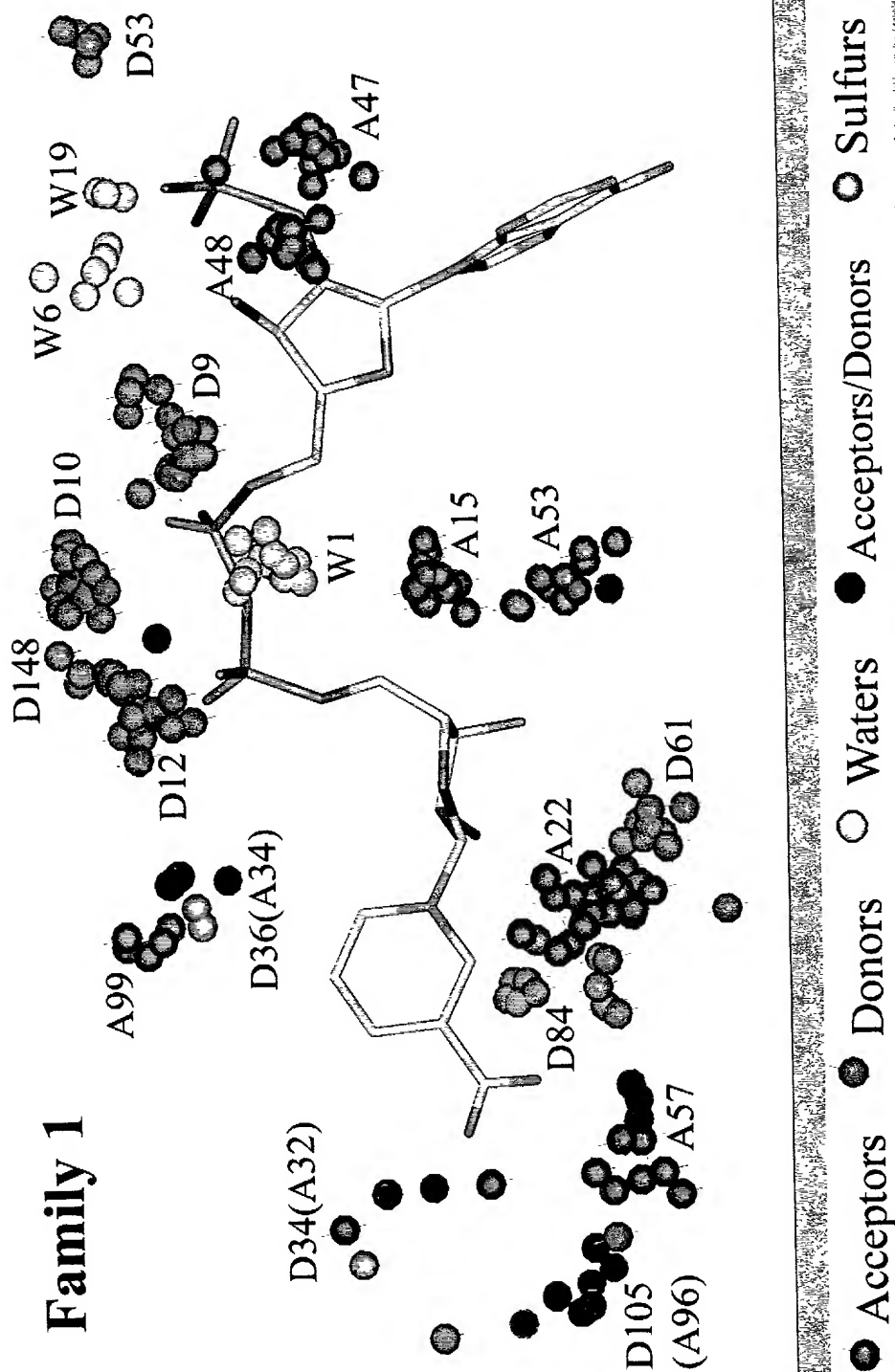
Pharmacocluster 7

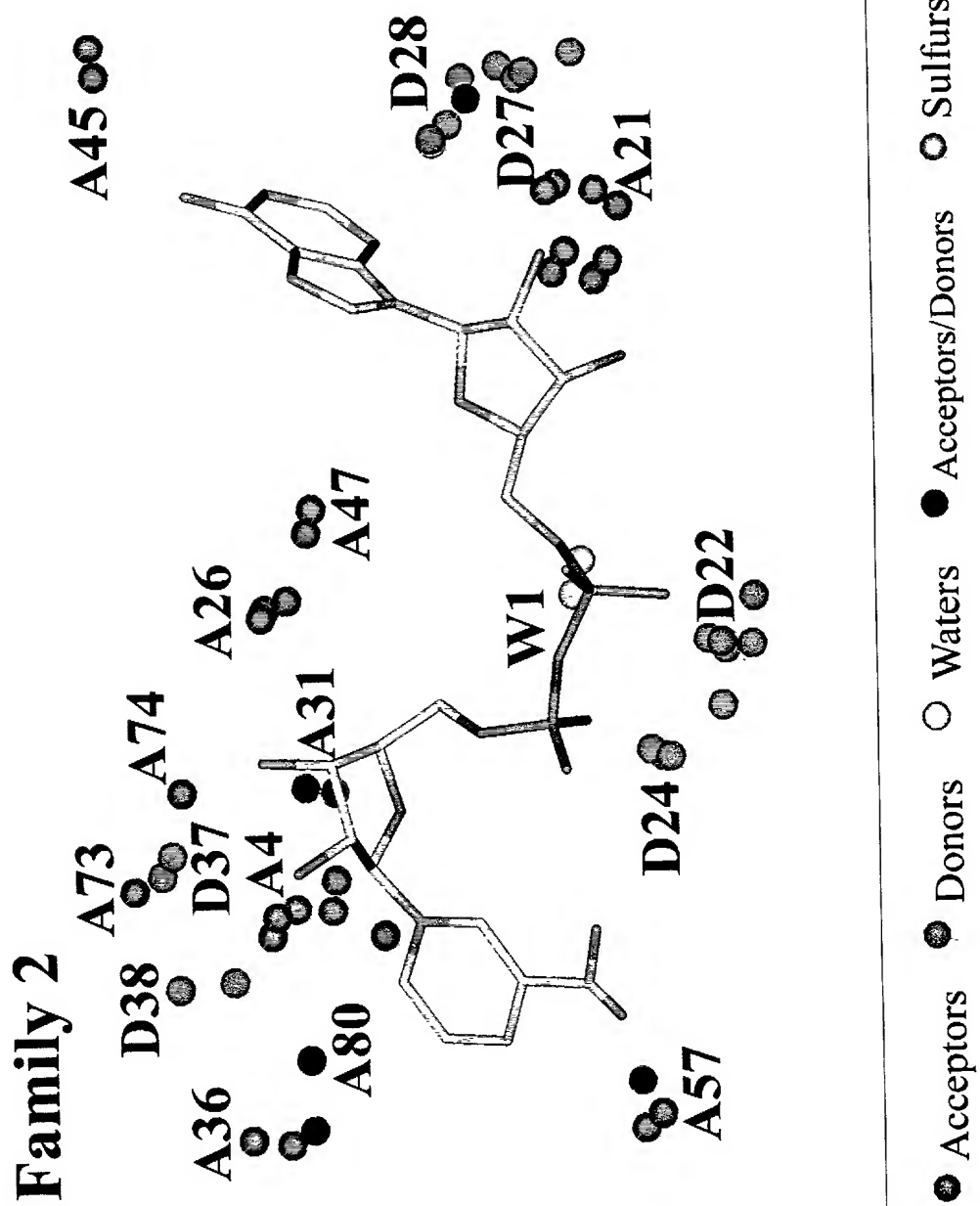


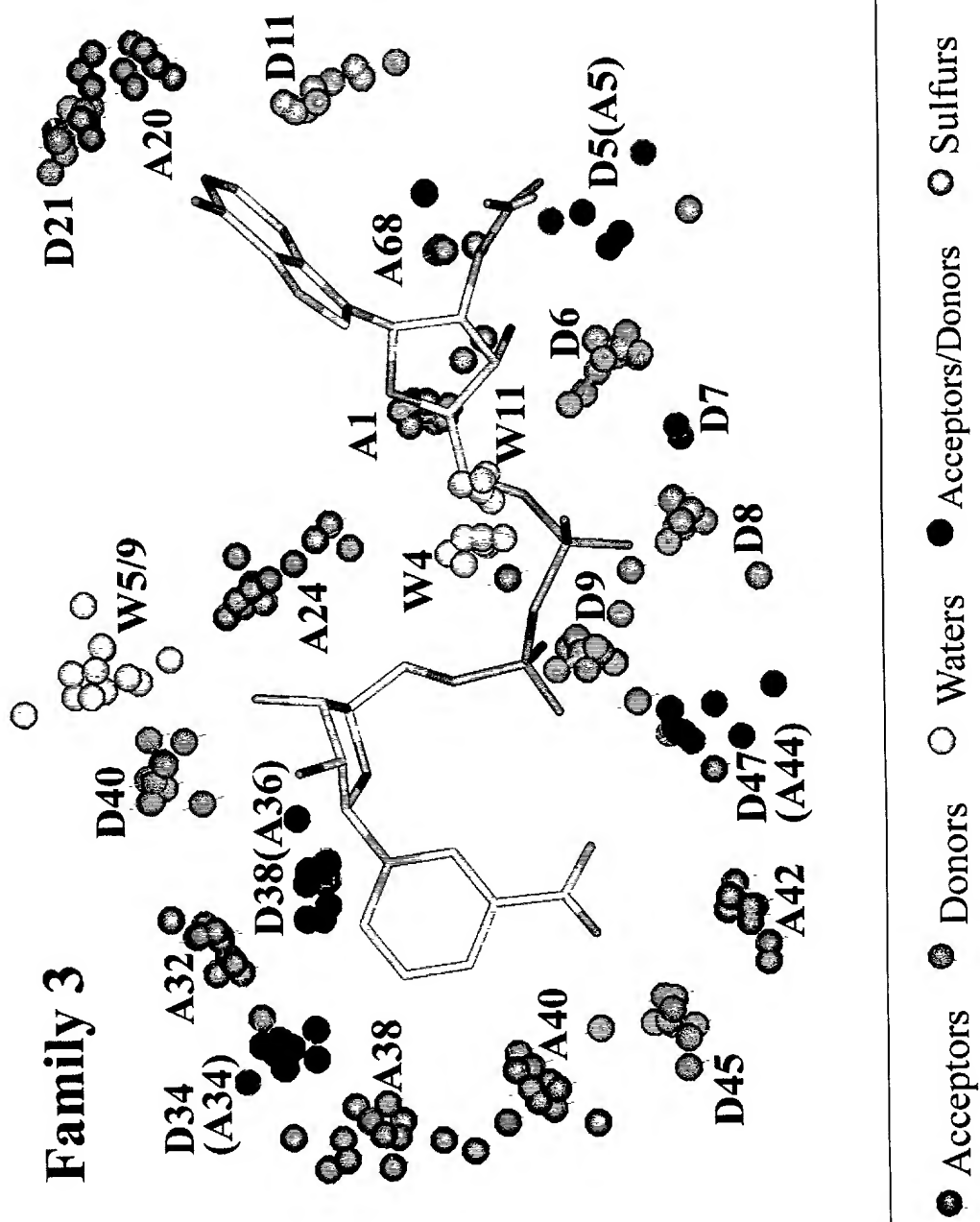
Pharmacocluster 8

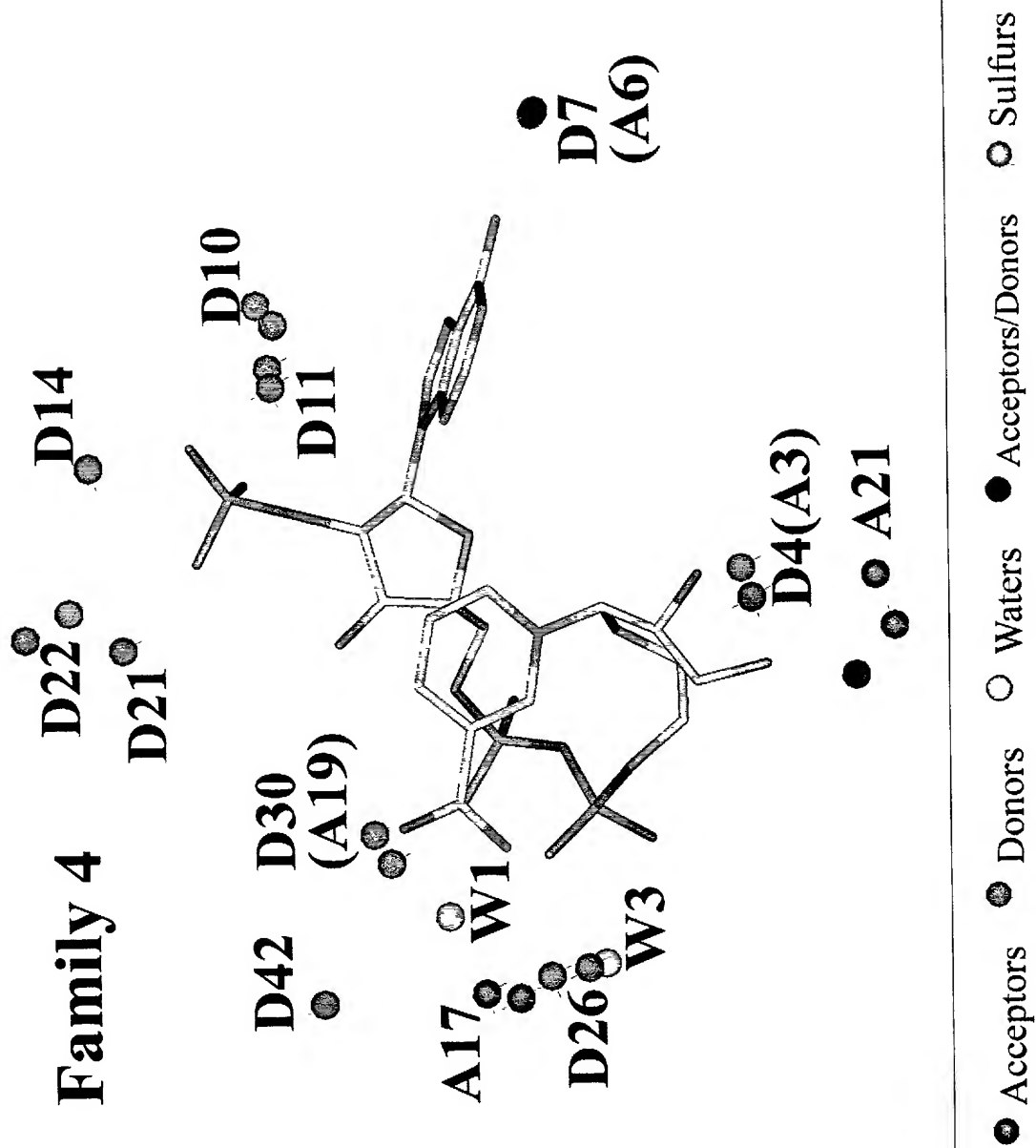
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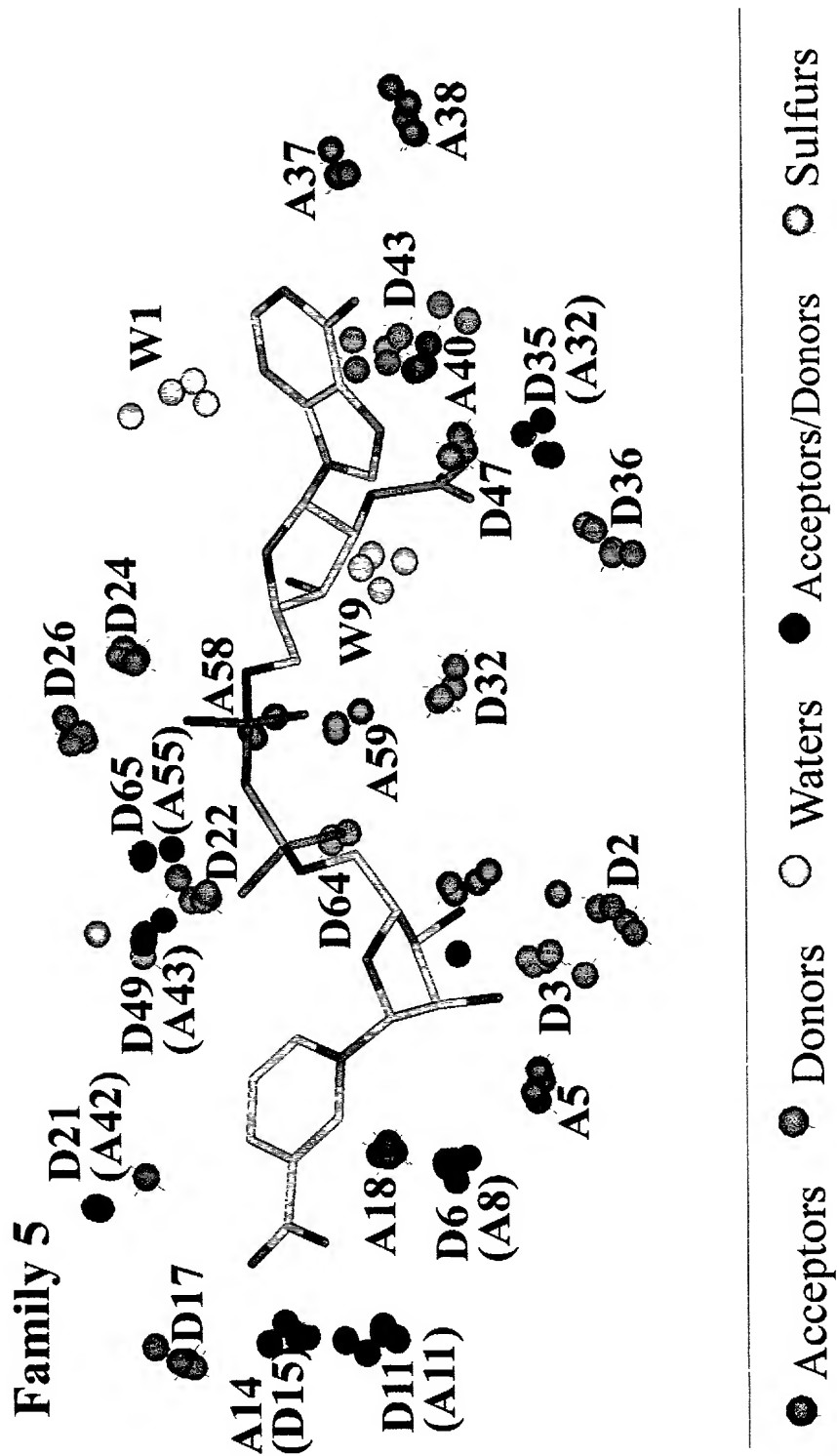


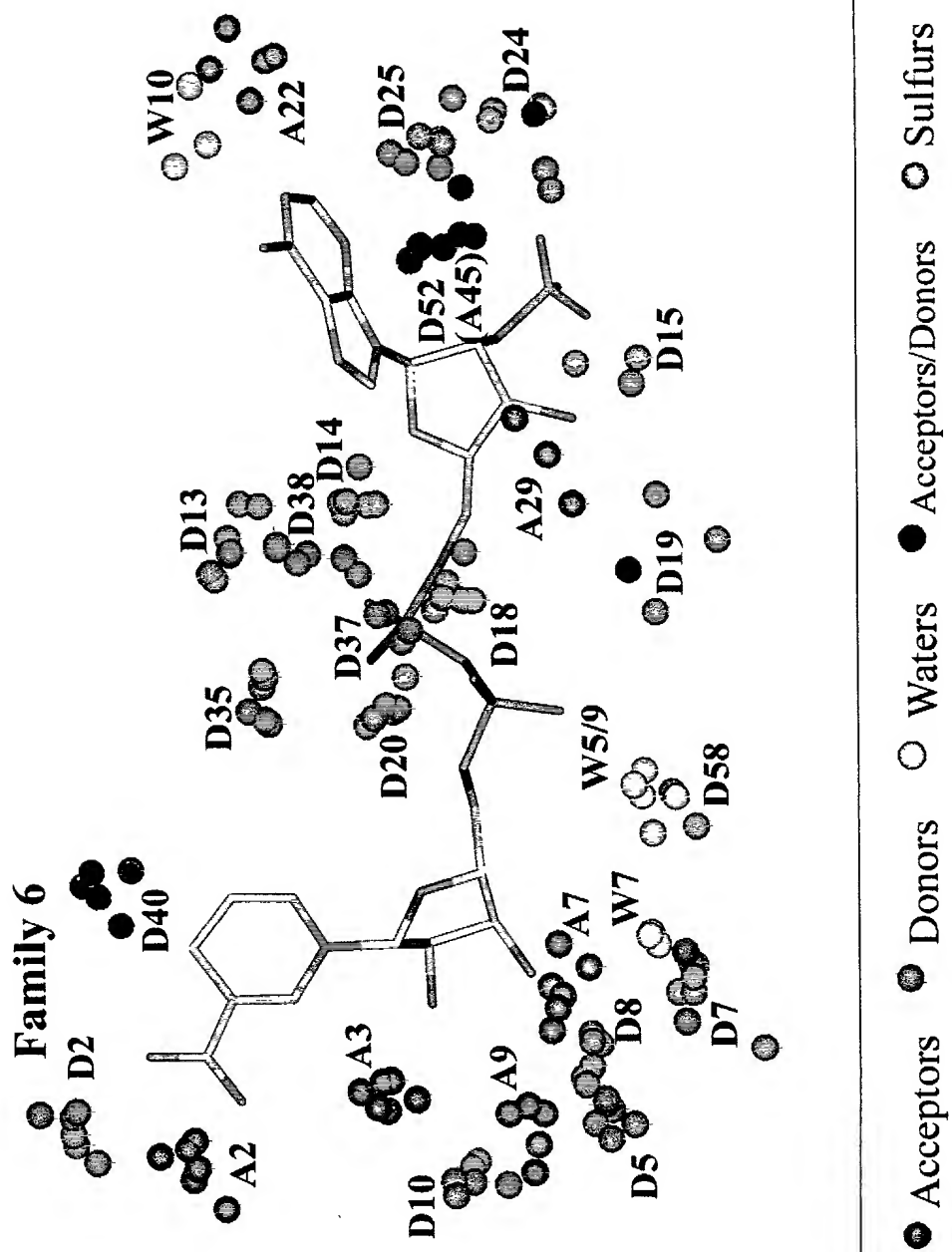




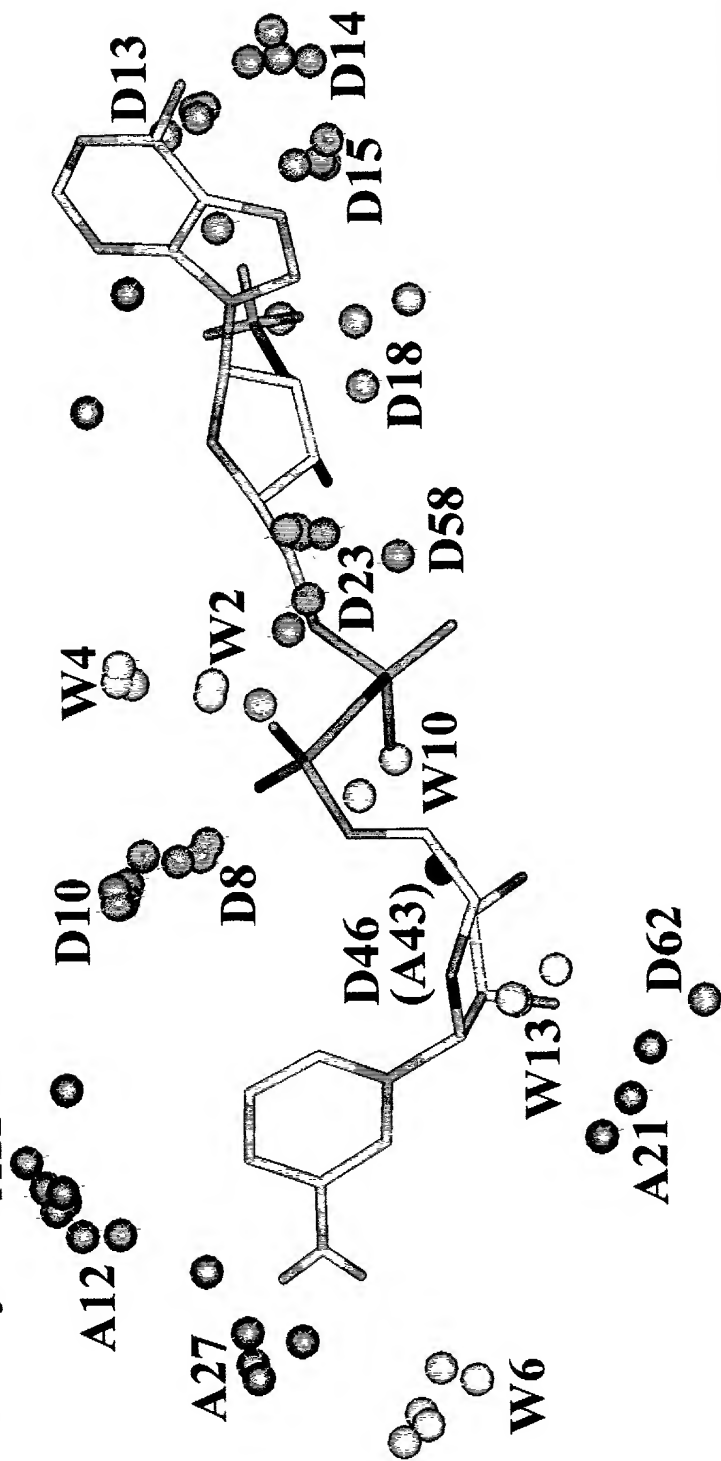




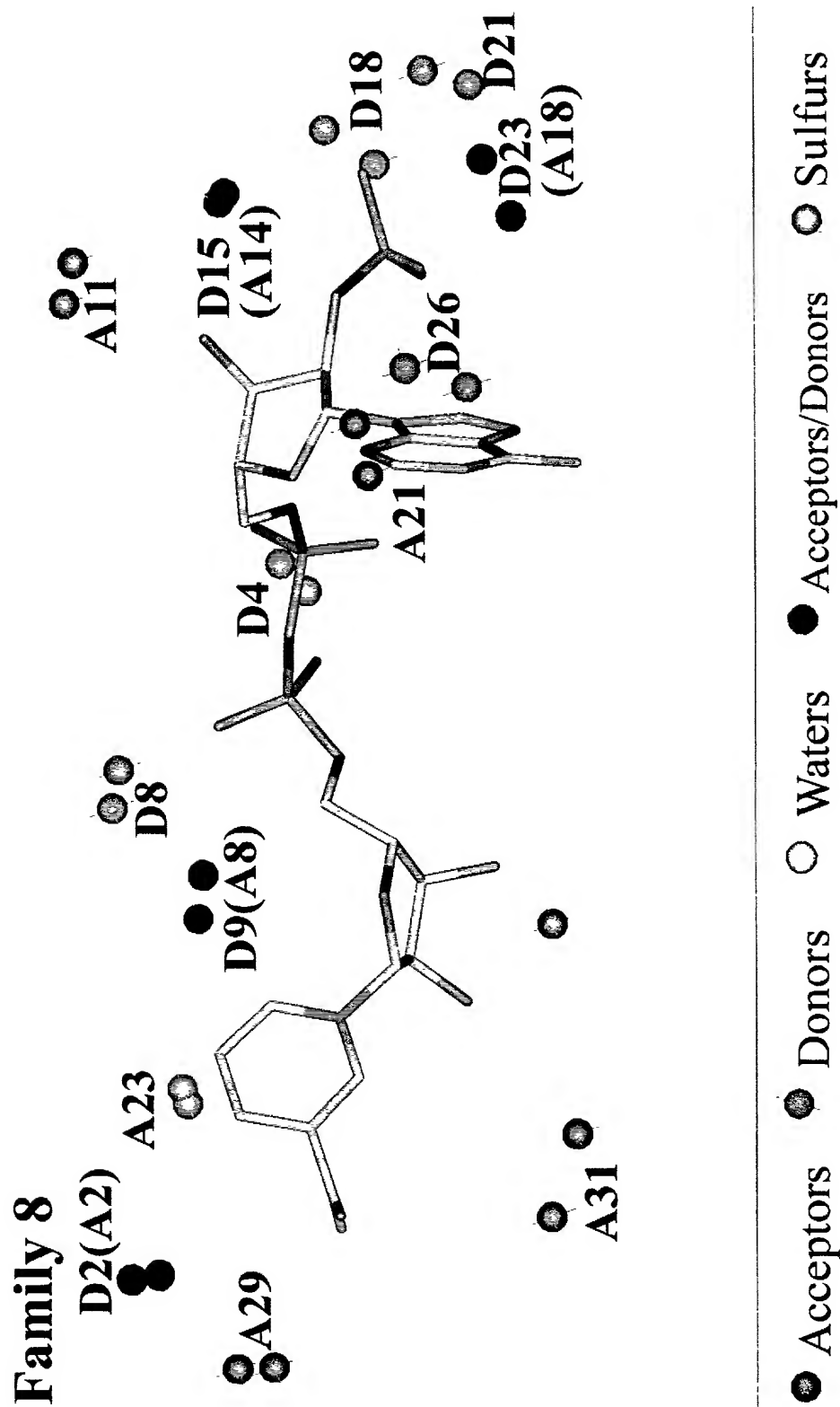


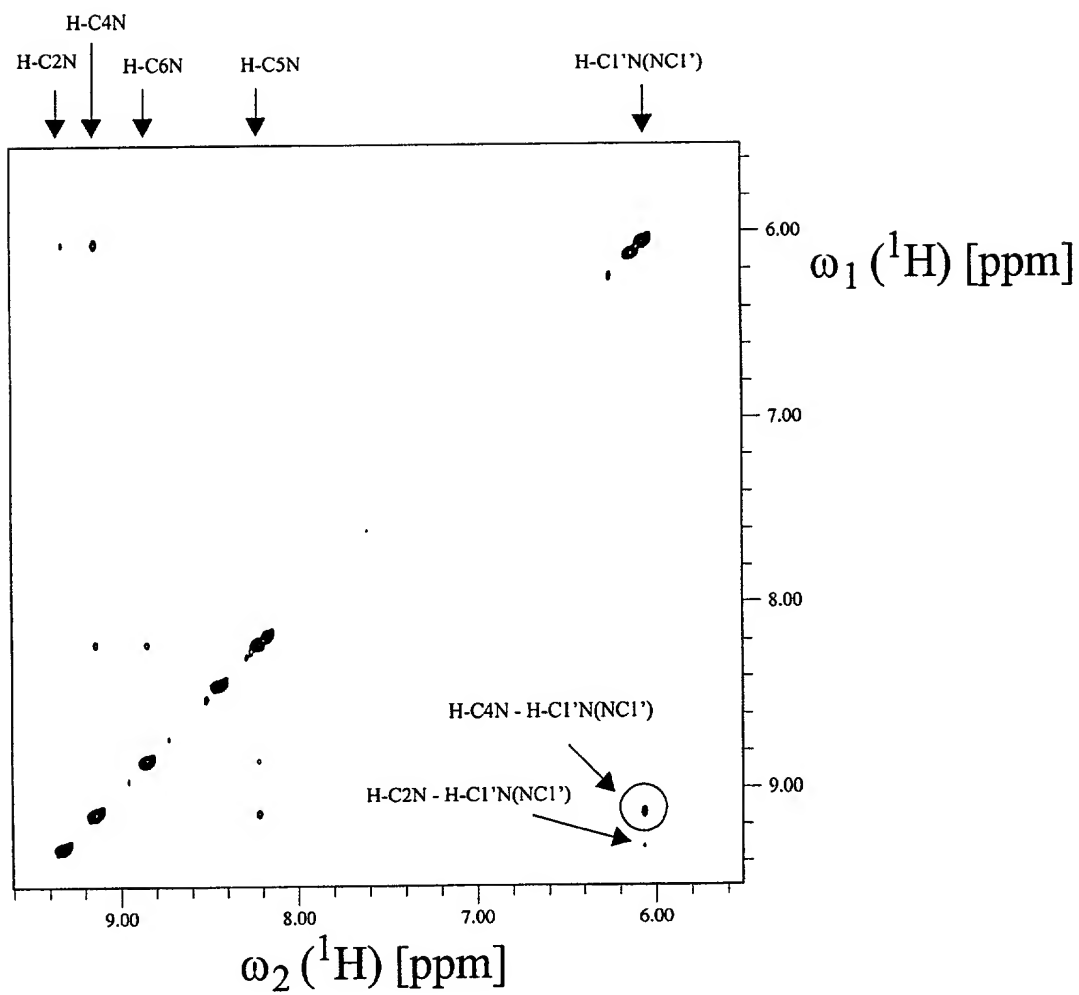


Family 7 A11

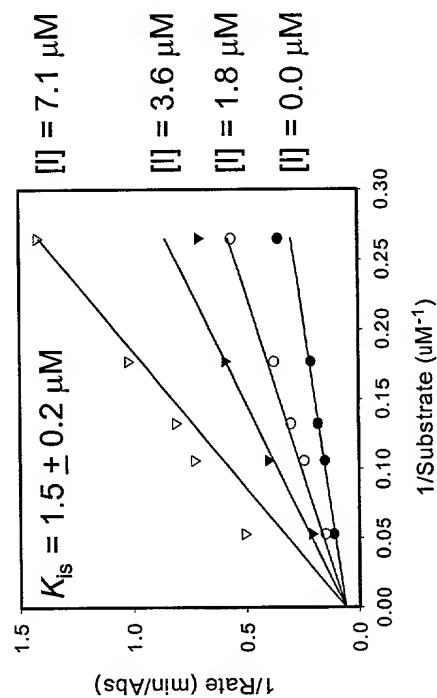


- Acceptors
- ◐ Donors
- Waters
- Acceptors/Donors
- Sulfurs

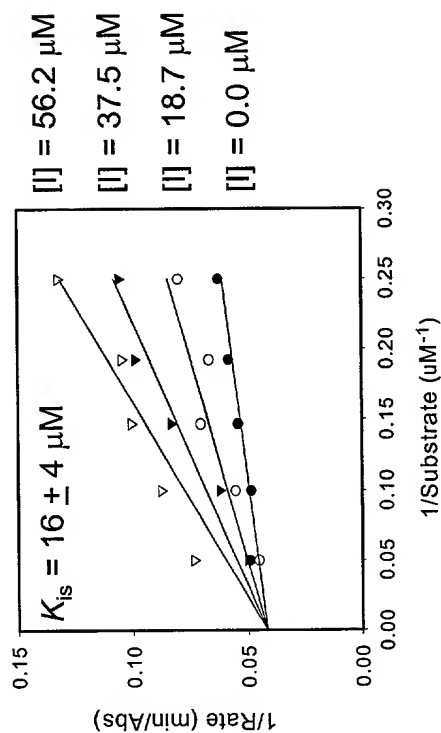




A.
Compound: TTE0001.001.A7
Pharmacofamily 1 exemplar

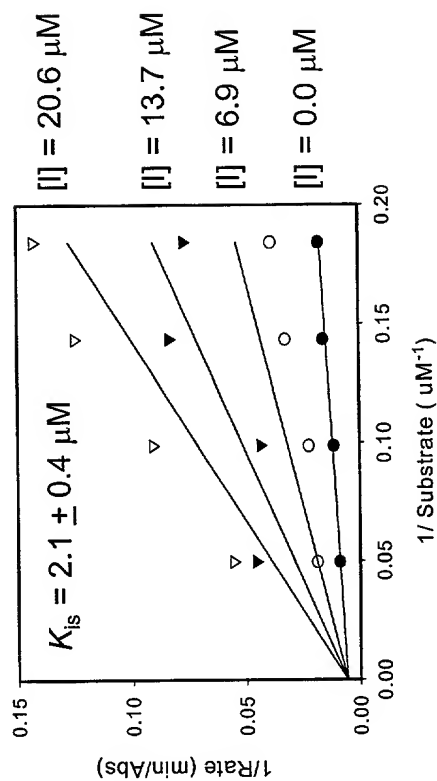


B.
Compound: TTE0001.001.A7
Pharmacofamily 8 exemplar

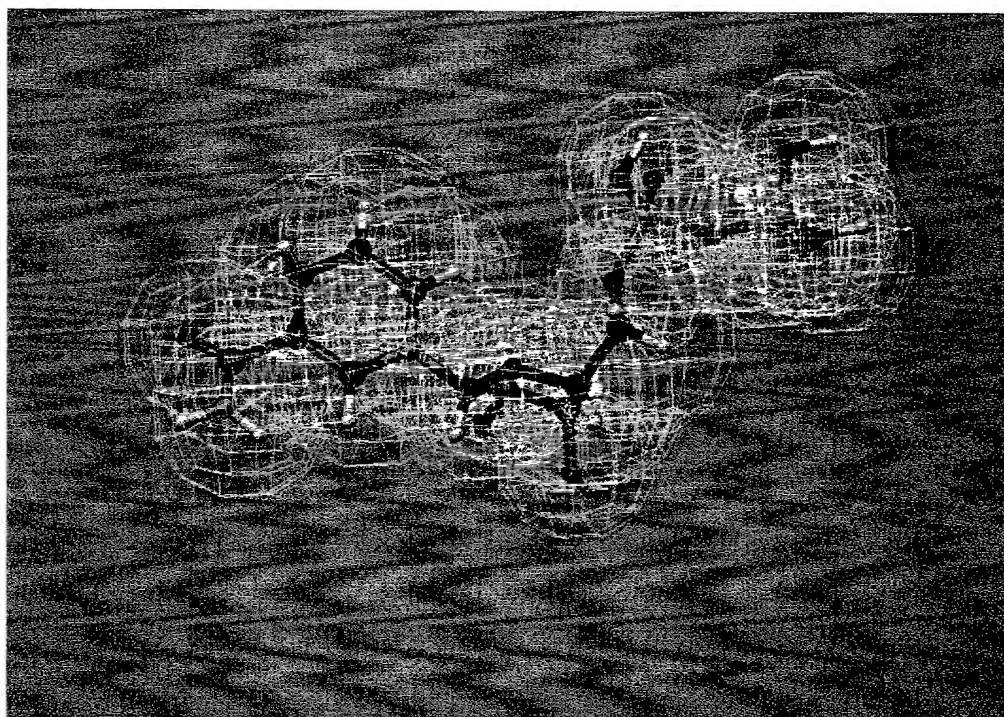


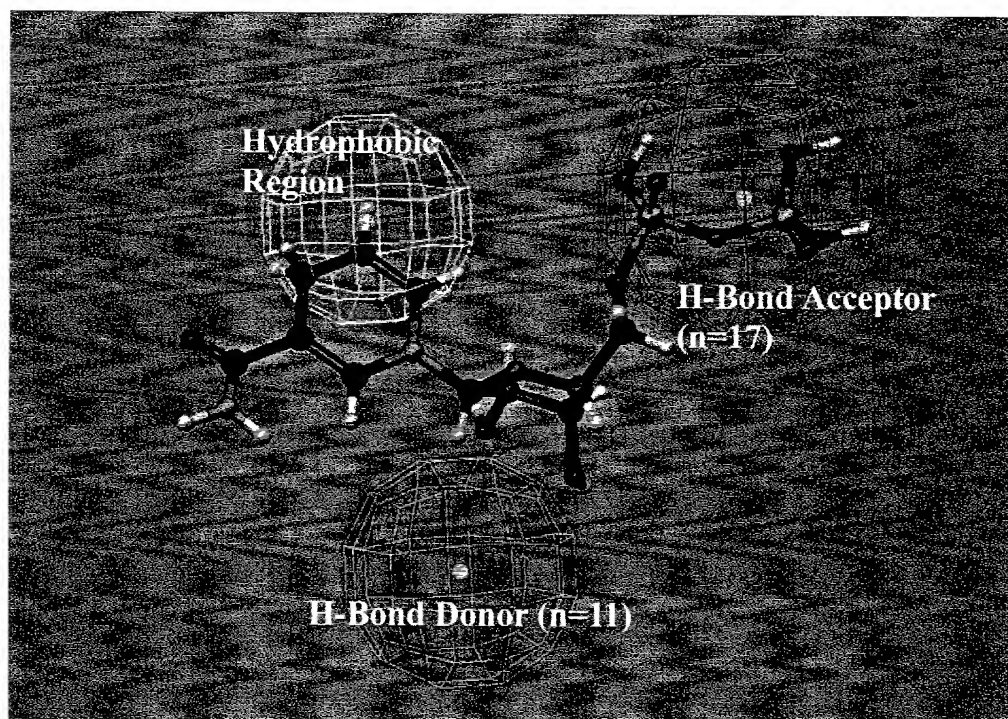
B.
Compound: TTE0001.002.D2
Pharmacofamily 8 exemplar

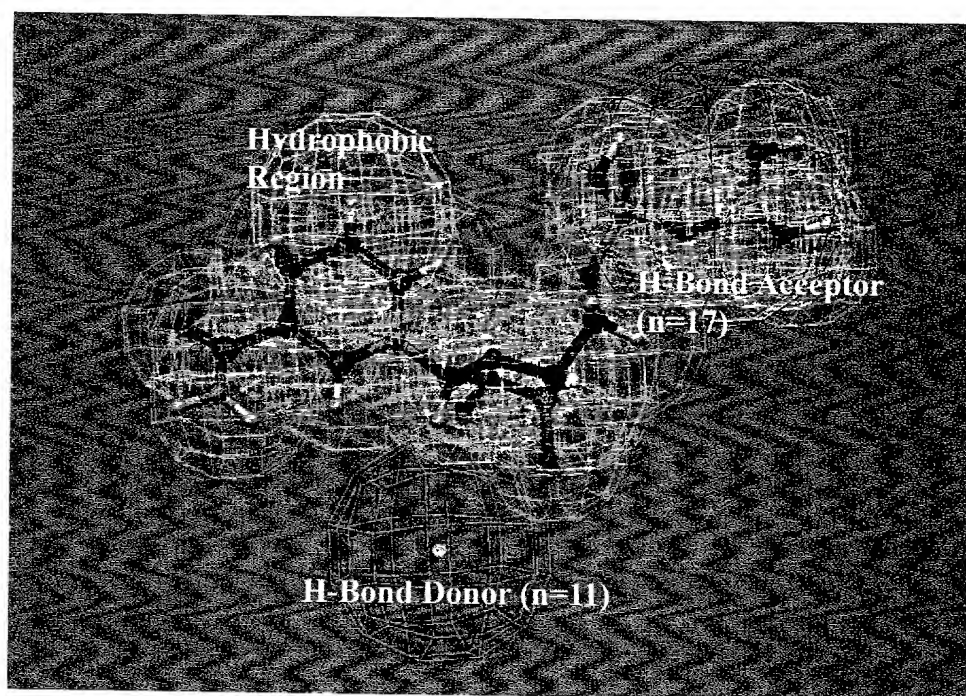
A.
Compound: TTE0001.002.D2
Pharmacofamily 1 exemplar



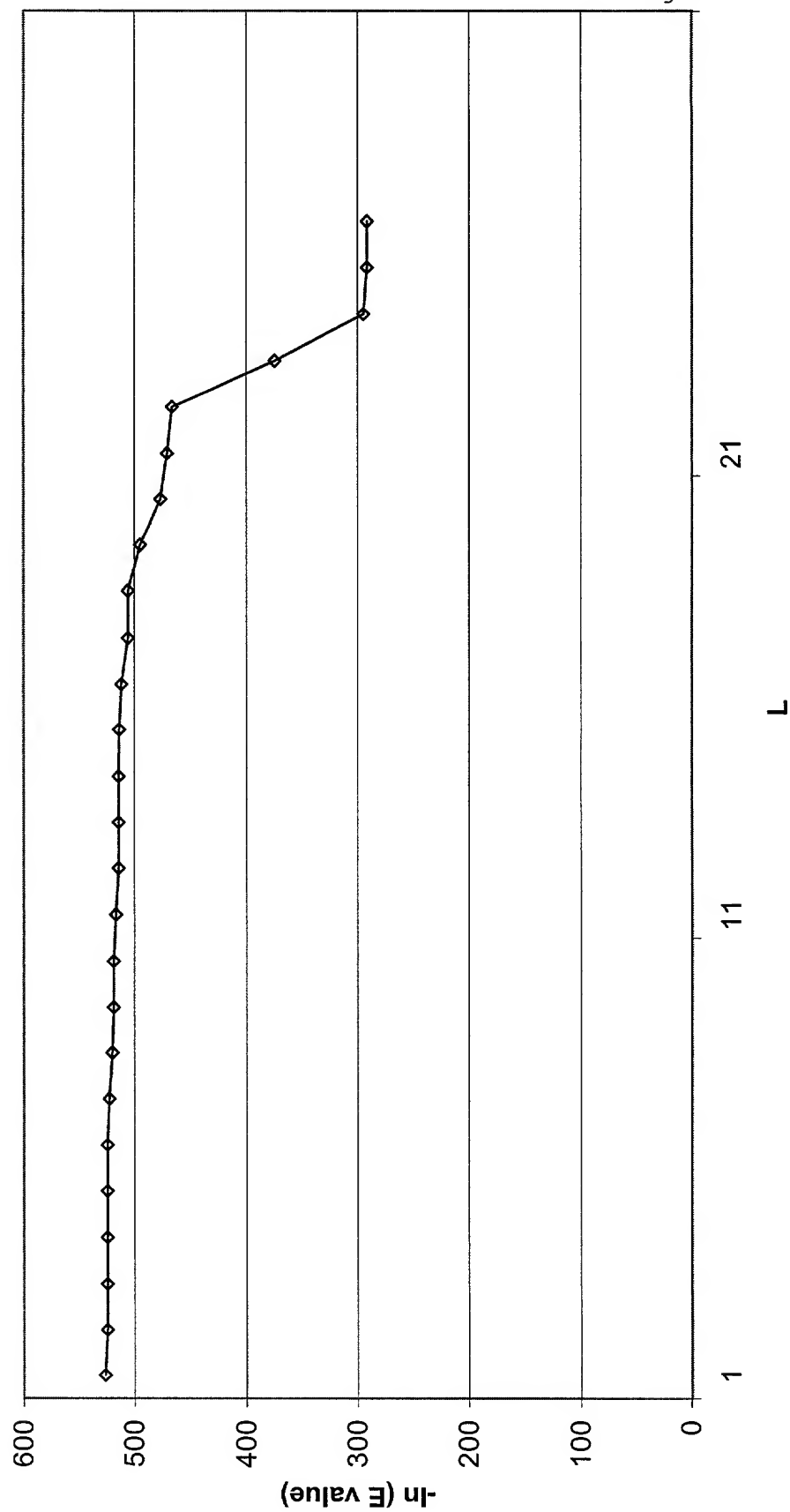
$K_{is} > 1 \text{ mM}$



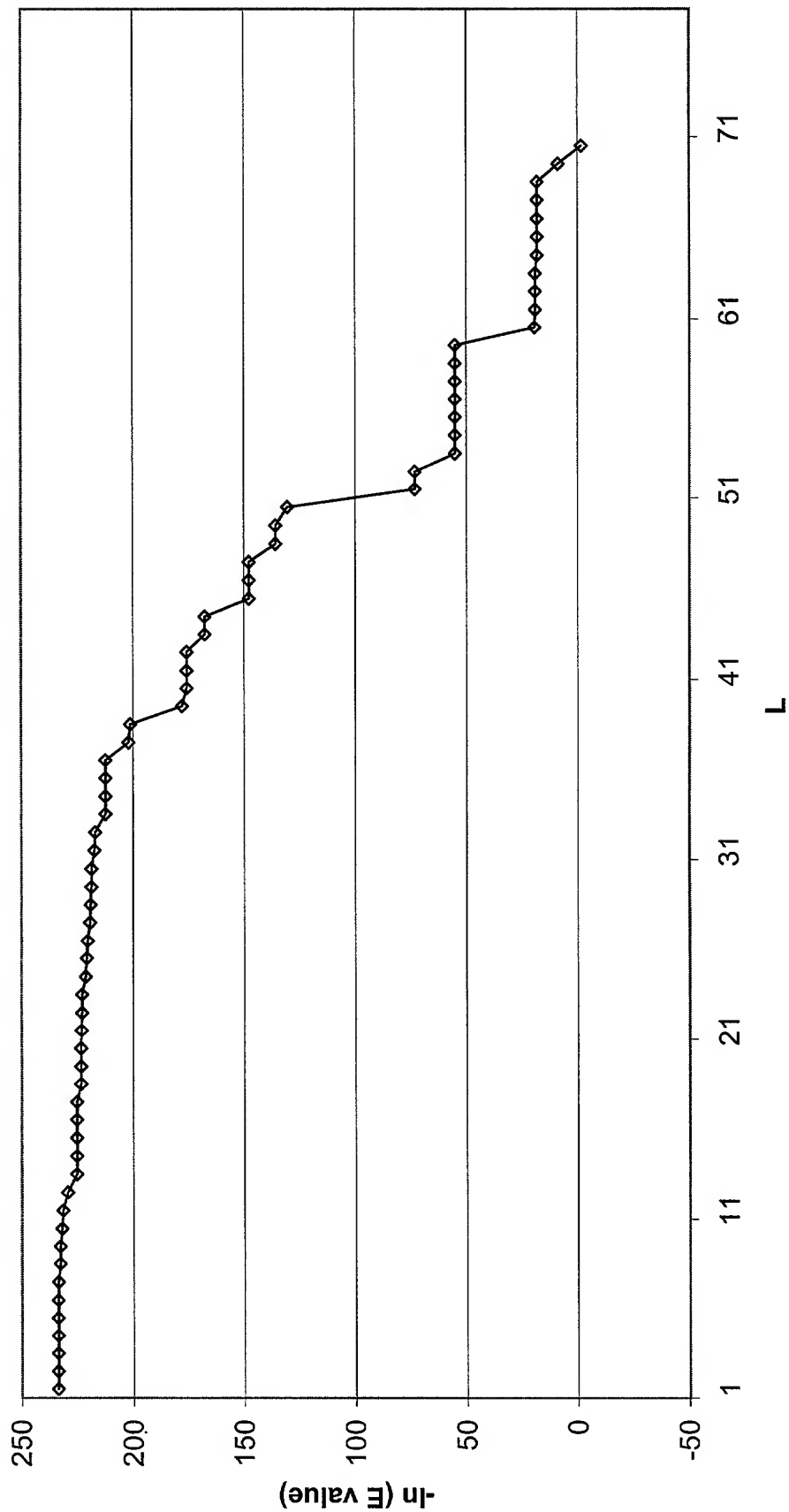




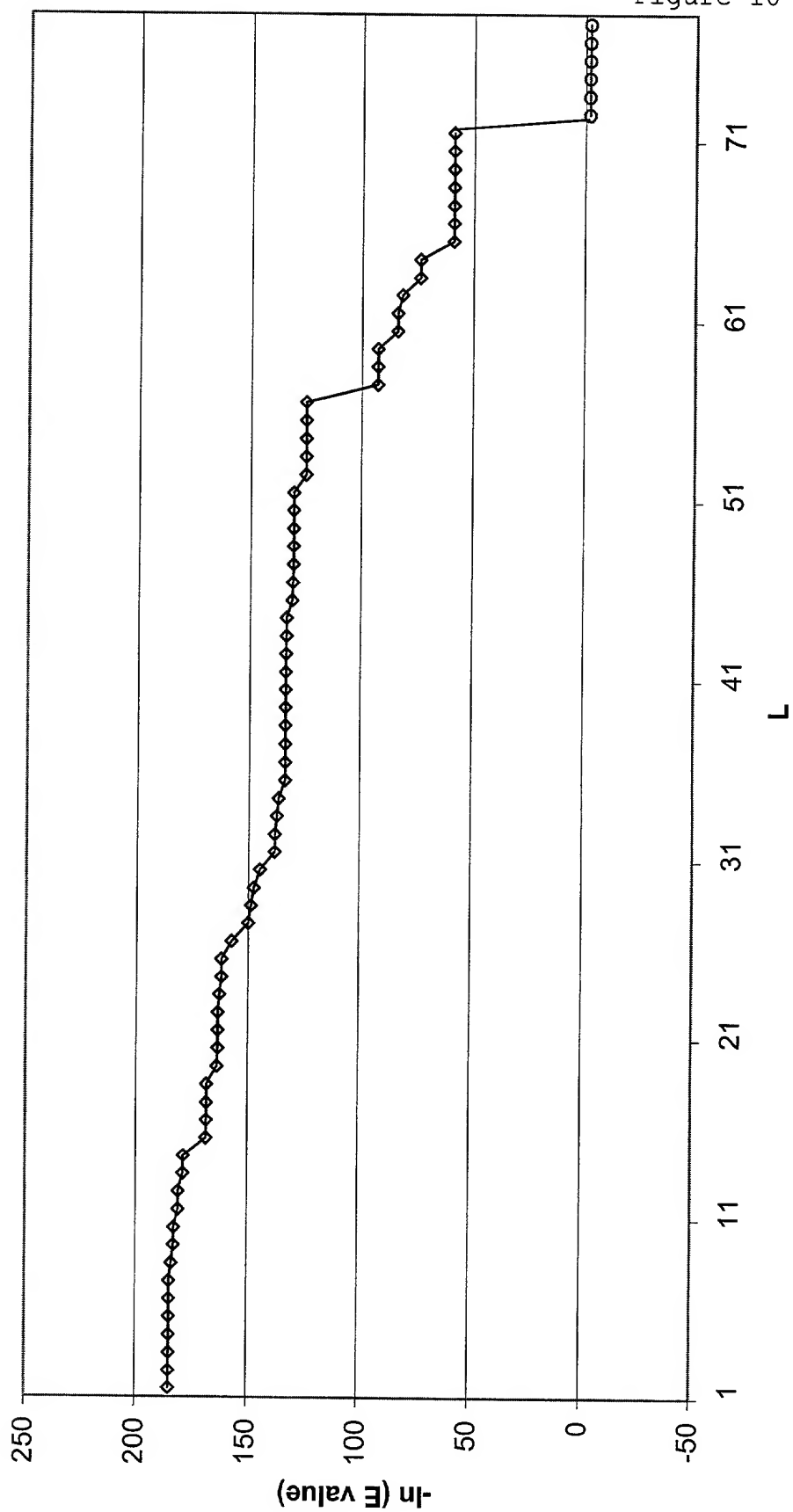
Pharmacofamily 5



Pharmacofamily 3 : Training Set 1



Pharmacofamily3 : Training Set 2



refinement cycle 5
profile center:1AGN
profile length: 599

1AGN
1AXE
1YKF
1HYH
1LDN
1EMD
9LDB
4MDH
1BMD
1PSD
1DXY
2NAD
1A4I
1B3R
1PJC
1ARZ
1QR6

1AGN:CL.....	IGC.	.GFSTGYGAA	VKTGK...V.
1AXE:	GC.	.GFSTGYGSA	VKVAK...V.
1YKF:VM.....	IPD.	.MMITGFHGA	E.LAD...I.
1HYH:
1LDN:
1EMD:
9LDB:ATLKDQL.	I.HNL...L.
4MDH:
1BMD:
1PSD:P.....	..F.....	SN.	.TRSV AELV.	IGELL.LLLR
1DXY:	...SNV....	..P.....	AYS.	.PAAIAEFA.	LTDTL.YLLR
2NAD:	CN.	.SISVAEHV.	VMMIL.SLVR
1A4I:PCTPKGC.	LELIK.ET.G
1B3R:	KFD.	NLYGCRESL.	IDGIKRAT.D
1PJC:	TPM	SI.IAGRLSV	Q.FGA.RFLE
1ARZ:
1QR6:	LIQFEDFGNH	NAFRFLRK <u>YR</u>	EKYCTFNDD.IQGTAAVA.	LAGLL.AAQK

1AGN:KP.....	.G.STCVVF.
1AXE:TQ.....	.G.STCAVF.
1YKF:EL.....	.G.ATVAVL.
1HYH:A.RKIGI <u>IG</u>
1LDN:MK...NN	GG. <u>ARVVVIG</u>
1EMD:MKVAVL <u>G</u>
9LDB:KEE...HV	PH.NKITV <u>VG</u>
4MDH:SE.....	.P.IRVLV <u>TG</u>
1BMD:MKA.....	.P.VRVAV <u>TG</u>
1PSD:	..GVPEANAK	A..HRGV.W.	NKL..AA.G.	SFEAR.....G.KKLG <u>II</u> .
1DXY:	..NMGKVQAQ	L..QAGDYEK	AGT..F..I.	GKELG.....Q.QTVGV <u>M</u> .
2NAD:	..NYLPSHE.	WARK.GGWN.	.IADCVSHA.	Y.DLE.....A.MHVGT <u>V</u> .
1A4I:VPIA.....	.G.RH <u>AVVV</u> .
1B3R:VMIA.....	.G.KVAVV <u>A</u> .
1PJC:	RQQ.....	GGR	GVLLGGVPGV	KP.GKVVIL.
1ARZ:N.....	...IRVAI <u>AG</u>
1QR6:	..V.....	I.	SKP.I.....	.SEHKIL <u>FL</u> .

1AGN: GLGG.VGLSV IMGCK..SA.G... .A.SRIIGID ..L.N.....
1AXE: GLGG.VGLSV IMGCK..AA.G... .A.ARIIGVD ..I.N.....
1YKF: GIGP.VGLMA VAGAK..LR.G... .A.GRIIAGVS.....
1HYH: L.GN.VGAAV AHGLIAQGV. .A..... .D..DYVFD A.N.E.....
1LDN: A.GF.VGASY VFALMNQGI. .A..... .D..EIVLID A.N.E.....
1EMD: AAGG.IGQAL ALLLKTQLP. .S...G... .S..ELSLYD I.A.P.....
9LDB: V.GA.VGMAC AISILMKEL. .A..... .D..EIALVD V.M.E.....
4MDH: AAGO.IAYSL LYSIG.NG.S VFGKDQP... .I..ILVLLD ITP.MM....
1BMD: AAGO.IGYSL LFRIA.AG.E MLGKDQP... .V..ILQLLE I.POAM....
1PSD: GYGH.IGTQL GILAE..SL.G... .M..YVYFYD I..E.....
1DXY: GTGH.IGQVA IKLFK..GF.G... .A..KVIAVD P..Y.....
2NAD: AAGR.IGLAV LRRLA..PF.D... .V..HLHYTDR.....
1A4I: GRSKIVGAPM HDLLL..WN.N... .A..TVTTCH S..K.....
1B3R: GYGD.VGKGC AQALR..GF.G... .A..RVIITE I..D.....
1PJC: GGGV.VGTEA AKMAV..GL.G... .A..QVQIFD I..N.....
1ARZ: AGGR.MGRQL IQAAL.ALE. GV..... .Q..LGAALF REG.SS....
1QR6: GAGE.AALGI ANLI...VS. ..VENGLSEQ EAQKKIW.FD K..YGLLVK

1AGN: ...KD.KFEK AM.AVGA... ..T.E.C...I
1AXE: ...KD.KFAK AK.EVGA... ..T.E.C...V
1YKF: ...RPVCVDA AK.YYGA... ..T.D.I...V
1HYH: ...A..KVK. .A.D.QID.. FQ.....DAM ANL.EAH.G. NI.V.I...N
1LDN: ...S..KAI. .G.D.AMD.. FN.....HGK V.FAPKP.V. DI.W.H...G
1EMD: ...V...TP. .G.V.AVD.. LS.....HI. .P..TA.V. KI.K.G...F
9LDB: ...D...KLK. .G.E.MMD.. LQ.....HGS L.F..LR.TP KI.V.S...G
4MDH: ...G...VLD. .G.V.LME.. L.....QDC .A..LPLLK DV.I.A...T
1BMD: ...K..ALE. .G.V.VME.. LE.....DCAFPLLA GL.E.A...T
1PSD: ...N..K... .L...P.... LG..... NA.T.Q...V
1DXY:P... .M.K.GD... HP..... DF.D.Y...V
2NAD: ...H..R... .L.P..ES.. VE.....KE..L. NL.T.W...H
1A4I:
1B3R: ...PI..NAL. .Q.A.AM... EG..... .Y.E.V...T
1PJC: ...VERL... .SYL..ETL. FG.....SRV.ELL...Y
1ARZ: ...L...LG. .S.D.A.... GELAGAGK.TGV.T.V...Q
1QR6: GRKAK..... .I.D...SYQ EP..... .FTHSAPESI

1AGN: S...PKDSTK PI.S.EVLSE M.T..G.NNV GYTFEVIG.. ...H.....
1AXE: N...PQDYKK PI.Q.EVLTE M.S..N.GGV DFSFEVIG.. ...R.....
1YKF: N...YKDG.. PI.E.SQIMN L.T..EGKGV DAATAGG.. ...N.....
1HYH:D..... .W....A. .ALAD...A DVVISTLG.. ...NIKLOQ..
1LDN:D..... .Y....D. .DCRD...A DLVVICAG.. ...AN..OKP..
1EMD: SGE.D..... .A.T.PAL.. .E.G...A DVVLISAG.. ...VR..RK..
9LDB: K...D..... .Y..NVT.. .A.N...S RLVVITAG.. ...AR..QQE..
4MDH: D...K..... .EEI..AFK. .D.....L DVAILVGS.. ...MP..RR..
1BMD: D.D.P..... .D.V..AFK. .D.....A DYALLVGA.. ...AP.RKA..
1PSD: Q.H.L..... .S.D..LLN. .M.....S DVVSLHVPEN PST.....
1DXY: S...L..... .E.D..LFK. .Q.....S DVIDLHVPGI EQN.....
2NAD: AT..R..... .E.D..MYP. .V.....C DVVTLNCPLH PET.....
1A4I: TAH..L..... .D.E..EVN. .K.....G DILVVATG.. ...Q.....
1B3R: T...M..... .D.E..ACK. .E.....G NIFVTTG.. ...C.....
1PJC: SNSAE..... IE.T..AVA. .E.....A DLLIGAVLVP GRRRA.....
1ARZ: S...S..... .LDAV.K. .D.D....F DVFIDFT.. ...R.....
1QR6: PDT.F..... ED.A...VN. ILK.....P STIIGVAGA.. ...G.....

1AGN:L...ETM.I.DALA.SC....HMNYGT SVVVGV..P.
1AXE:L...DTM.V.TALS.CC....QEAYGV SVIVGV..P.
1YKF:A...DIM.A.TAVK.IV....KPGGT IANVNY..F.
1HYH:FA..E LKFTSSM.V.Q S..V.GTNLK .ESGFH..GV LVVISN.P..
1LDN: GET.RLD..L VDKNIAIF.R S..I.VESVM .ASGFQ..GL FLVATN.P..
1EMD: PGMDRSD..L FNVNAGIV.K N..L.VQQVA .KT.CP.KAC IGIITN.P..
9LDB: G.ESRLN..L VQRNVNIF.K F..I.IPNIV .KY.SP.NCK LLVVSN.P..
4MDH: DGMERKDL.L .KANVKIF.K C..Q.GAALD .KY.AKKSVM VIVVGN.P..
1BMD: .GM..ERRDL LQVNGKIF.T E..Q.GRALA .EV.AKKDVK VLVVGN.P..
1PSD:K..NM.M GAKE.ISLM.KP.GSL LINASR.GT.
1DXY:T..HI.I NEAA.FNLM.KP.GAI VINTAR.PN.
2NAD:E..HM.I NDET.LKLF.KR.GAY IVNTAR.GK.
1A4I:P..EM.V ...K.GEWI.KP.GAI VIDCGI..N.
1B3R:V..DII ...L.GRHFE .Q..MKDDAI VCNIGH.F..
1PJC:P..I.L ...VPASLVE .Q..MRTGSV IVDVAV..DO.
1ARZ:P..EGTL N..H.LAFCR .Q..HG..KG MVIGTT..G.
1QR6:R..L.F TPDV.IR..A AS..INERPV IFALSNPTAQ

1AGN: .PSA.K.M.. .L.TY.D.PML...L...FT..
1AXE: .PDS.Q.N.. .L.SM.N.PML...L...LS..
1YKF: .GE..GEV.. .L....PVPRL EWGC..G...MA..
1HYH:V.D.. .V.I..TALFQH..V.....TG..
1LDN:V.D.. .I.L..TYATWKF.....SG..
1EMD:V.N.. .T.T..VAIAAEV.....LKKA
9LDB:V.D.. .I.L..TYVAWKI.....SG..
4MDH:A.N.. .T.N..CLTASKS.....AP..
1BMD:A.N.. .T.N..ALIAYKN.....AP..
1PSD: .V...V.D.. .I.PA.LCDAL...A...SK..
1DXY: .L...I.D.. .T.QA.MLSNL...K...SG..
2NAD: .L...C.D.. .R.DA.VARAL...E...SG..
1A4I: ..YKVV.G.. .D.VA.YD.EA....K...E...
1B3R:D.V.. .E.ID.VKW.LNEN. ..AVEKVNI KPQVDRYL..
1PJC:G.. .GCVETLHPT SHTQPTY... .E...V...
1ARZ:F.DEA GK.QA.IRDAA.....AD..
1QR6: AE...C.... .TAEEE.AYTLT... ..E...

1AGN:GR.T WK.....GC
1AXE:GR.T WK.....GA
1YKF:HK.T IK.....GG
1HYH:FPAHK VI..G...TGT.....
1LDN:LPHER VI..G...S.....
1EMD: GV...YDKNK LF..G...VTTL DI...IRSNT FVAEL..KGK
9LDB:FPKNR VI..G...SGC...N.....
4MDH: .S...IPKEN FS..C...LTRL DH...NRAKA QIALK..LGV
1BMD: .G...LNPRN FT..A...MTR.....
1PSD:H.LAG AA.....ID VFPTE...P. .ATNSD.... .PF.T..S..
1DXY:K.LAG VG.....ID TYEYETEDL.LN..LAKH. GSFKDPLW.D
2NAD:R.LAG YA.....GD VWFPQ...P. .A..... .PK.D..H..
1A4I:R.ASF IT..PVPGGVG..P.....
1B3R: .LKNGHRI.I LLAEG...RL V...N..L.....
1PJC:FGV.V HY..G...VP
1ARZ:I.A IV..F...A.A..N.....
1QR6:GRC LF..A...SG SP..F..... .G.P

```

1AGN: .....V. FGG.L...KS .....
1AXE: .....I. FGG.F...KS .....
1YKF: .....L. C...P...GG ..RLRME... R.LIDL....
1HYH: .....
1LDN: .....
1EMD: QPGE....VE V.PVIG.GHS G.V.TI..LP LLS.QVPG.. ...V...SF
9LDB: .....
4MDH: TS.D....DV KNVIIWGNHS S.T.Q...YP DVNHAKVKLQ AKEVGVYEAV
1BMD: .....LD .....
1PSD: .P.L...CE FDNVLLTPHI G.G.S...TQ EAQENI....
1DXY: .E.L...LG MPNVVLSPHI A.Y.Y...TE TAVHNMV... Y.FSLQ....
2NAD: .P.W...RT MPYNGMTPHI S.G.T.....
1A4I: .....M. TVA.M...LM .Q..S.....
1B3R: .....G.C. A.MGH...PS FV.....
1PJC: .....NM PGA.VPWTA. .....
1ARZ: .....F.. S.V.G...A. .S..S.....
1QR6: .V.KLTDGRV F..TPGQGN. NVY.I...FP GVALAVILCN TRHISD....

1AGN: .....
1AXE: .....
1YKF: ..... ..V..FYKR VDPS.K.L..
1HYH: .....
1LDN: .....
1EMD: T.E.QEV.AD LTKRIQNAGT EVVEAKAGGG SATLSMGQAA ARFGLS.LVR
9LDB: .....
4MDH: KDDSW.LKGE FITTVQORGA AVIKARK..L SSAMSAAKAI CDHV.RDI..
1BMD: .....
1PSD: .....
1DXY: ..... H.LVDFLTKG ETSTEVTG..
2NAD: .....
1A4I: .....
1B3R: .....
1PJC: .....
1ARZ: ..... R..MTFA NGAV.RSAL..
1QR6: ..... S..VFLE AA...KA...

1AGN: .....
1AXE: .....
1YKF: .....V. ....
1HYH: .....
1LDN: .....
1EMD: A.LQGEQGVV .....ECAYV EG.DG..QYA ..RFFS.QPL LLGKNGVEER
9LDB: .....
4MDH: W....F..GT PEGEFVSMGI ISDGNSYGVP DDLLYSFPVT IKD..KT.WK
1BMD: .....
1PSD: .....
1DXY: .....
2NAD: .....
1A4I: .....
1B3R: .....
1PJC: .....
1ARZ: WLSGKESGLF ...DMR... ..D. ....
1QR6: .....LT S..QLTD... ..EEL .....A

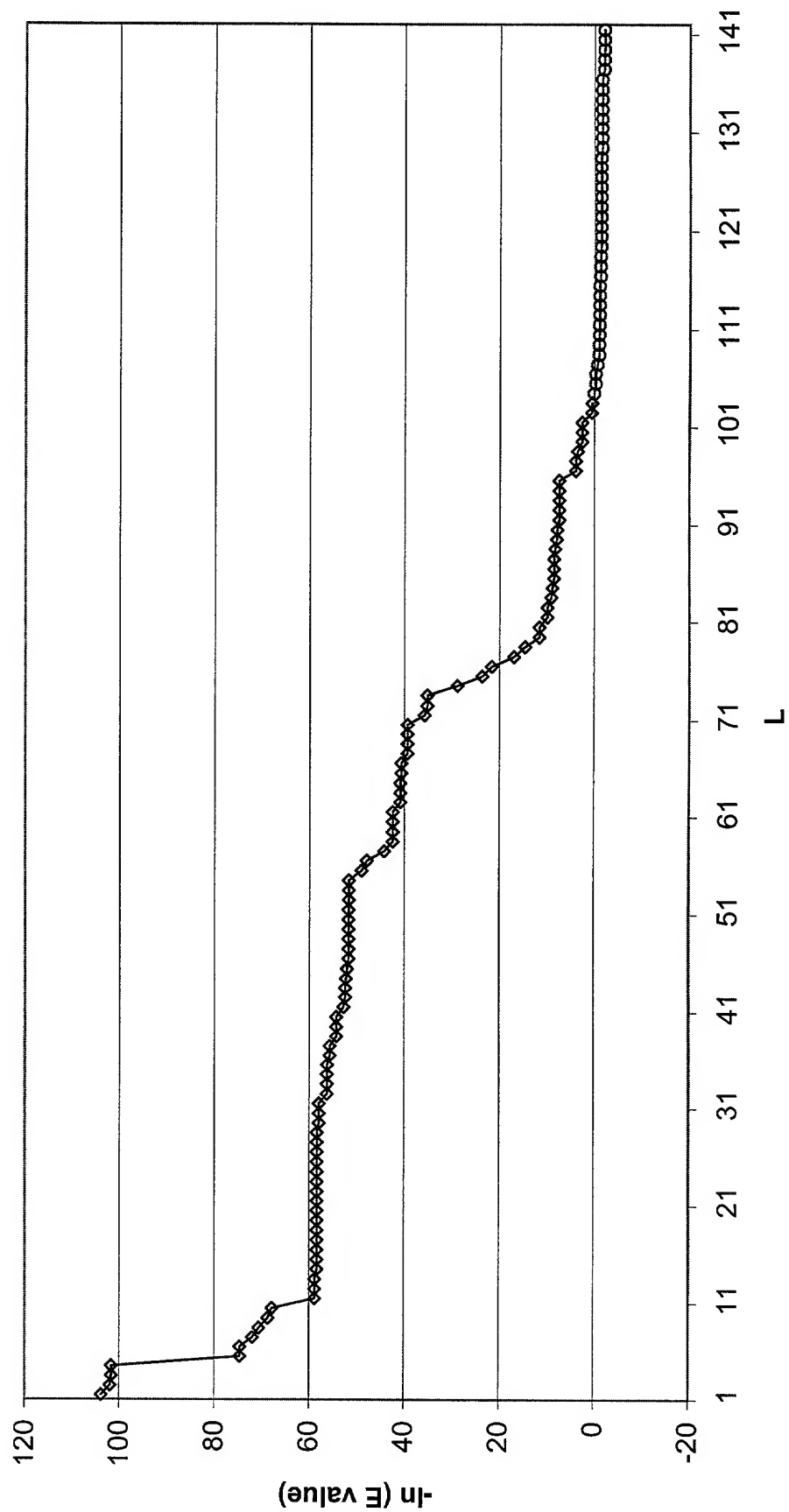
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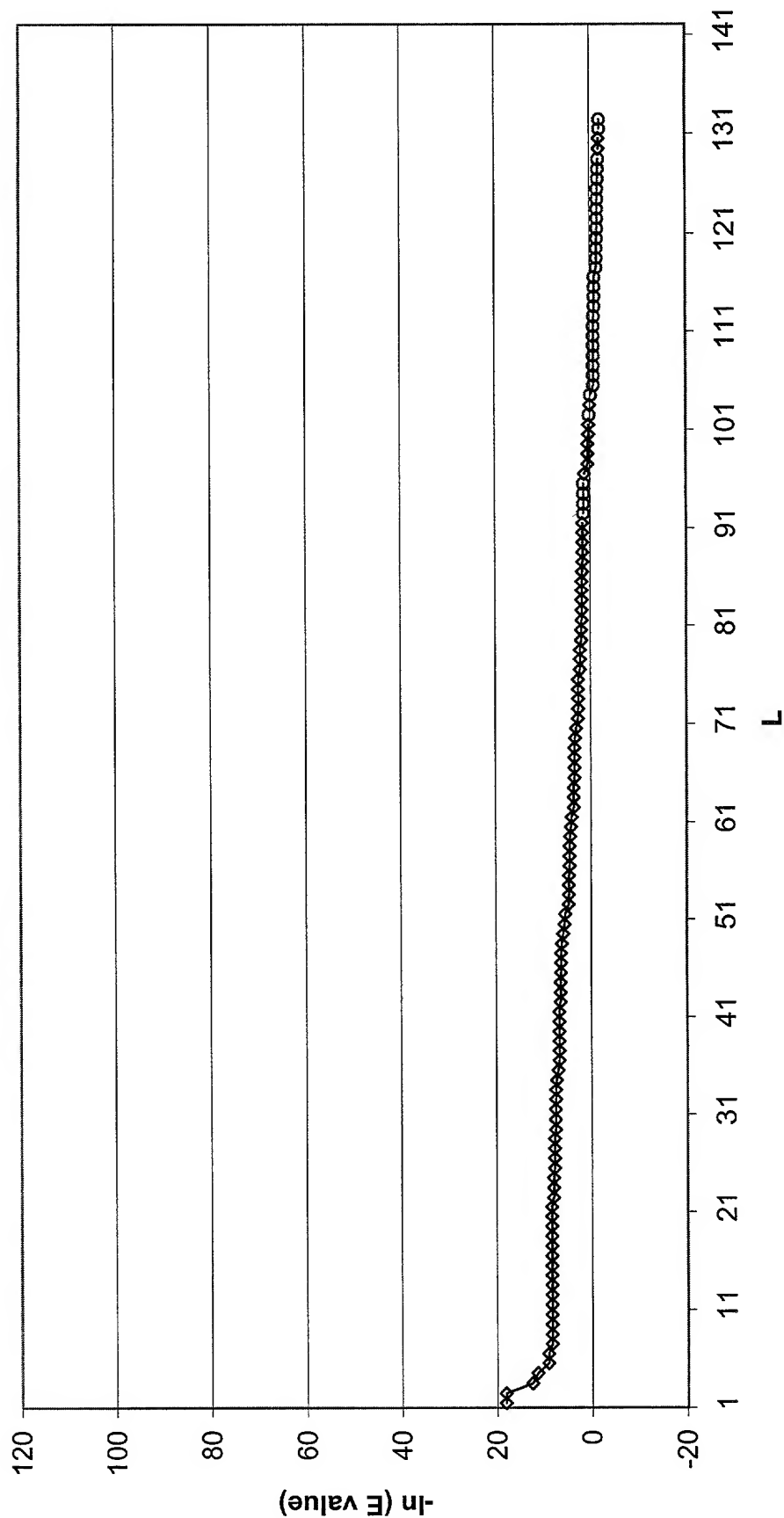
1AGN: .....
1AXE: .....
1YKF: .....
1HYH: .....
1LDN: .....
1EMD: K.S....I.G TLSAFEQNAL EG.ML...DT LKK.DIALGQ EF..VNK..
9LDB: .....
4MDH: I.V....EGL PI.N..DFS. REKMDLTAK L.AEE..KET AFEFL.SSA
1BMD: .....
1PSD: .....
1DXY: .....
2NAD: .....
1A4I: .....
1B3R: .....
1PJC: .....
1ARZ: ...VLDLN.N L.....
1QR6: QGRLYPPL.A NIQE.VSINI AIKVTEYLYA NKAFRYPEPE DKAKYVKER

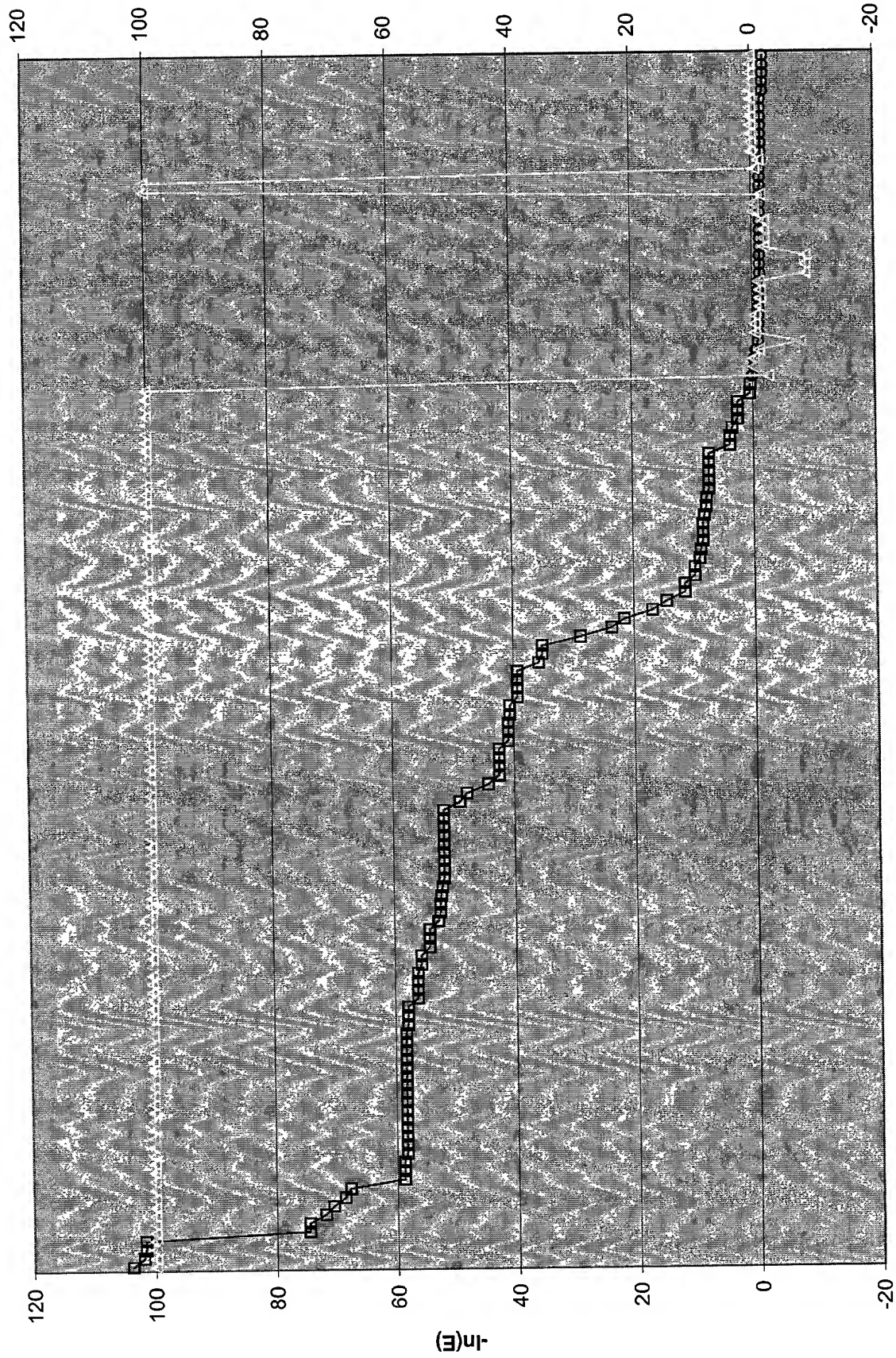
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Pharmacofamily 1



Pharmacofamily 1 with Differential Filtering





PDB Proteins for Pharmacofamily 1